Glenn T. Seaborg Center Special Seminar

Towards Predictive Modeling of Thermodynamic and Coordination Properties of Actinides

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Wednesday, January 8, 2014
4:00 pm – 5:00 pm
Bldg. 70A, Room 3377

Computational chemistry has reached the point where it makes significant contributions to the fundamental understanding of actinide chemistry, the interpretation of experimental data and the prediction of the physical behavior of actinides in the environment. Using unique heavy-element chemistry software capabilities in NWChem we explore the fundamental behavior of actinide species containing U, NP, Pu, and Cm in the gas phase and in aqueous environments. We will present some recent progress in modeling the structure, dynamics and thermochemistry of various complexes.

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